LLNL-PRES-748296

U.S. DEPARTMENT OF ENERGY | Office of Science

FASTMath: Frameworks, Algorithms and Scalable Technologies for Mathematics

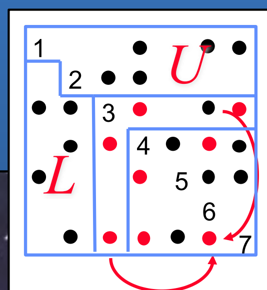
Lori Diachin, LLNL

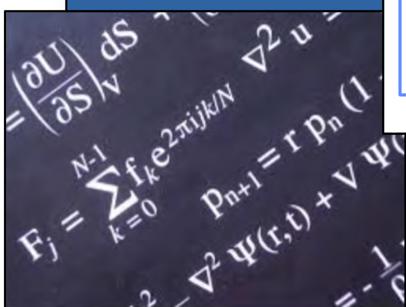
Institute Director

The FASTMath project brings leading edge computational mathematics technologies to the SciDAC Program

Develop advanced numerical techniques for DOE applications

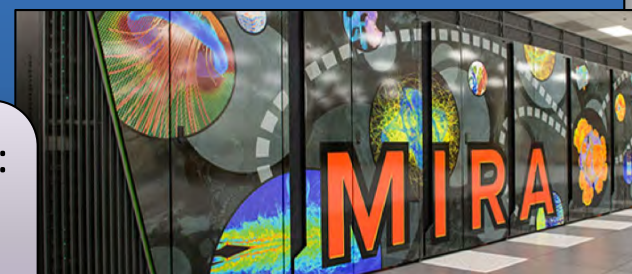
- Eight focused topical areas based on application needs
- High level synergistic techniques

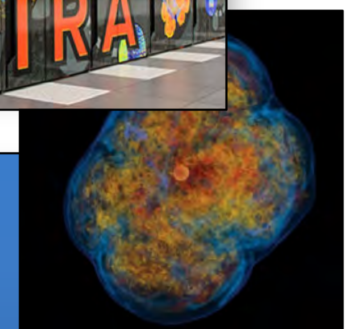




Deploy high-performance software on DOE supercomputers

- Algorithmic and implementation scalability
- Performance Portability
- Interoperability of libraries





FASTMath Objective: Reduce the barriers facing application scientists

Demonstrate basic research technologies from applied mathematics

- Build from existing connections with basic research
- Focus on research results that are most likely to meet application needs

Engage and support of the computational science community

- Publications and presentations in highly visible venues
- Team tutorials
- Workforce pipeline and training
- Web presence

The SciDAC-4 FASTMath Institute leverages and builds on the successes of SciDAC-3 to meet application needs

FASTMATH 3 + QUEST

+ Numerical Optimization

+ Data Analytics

=

FASTMATH 4

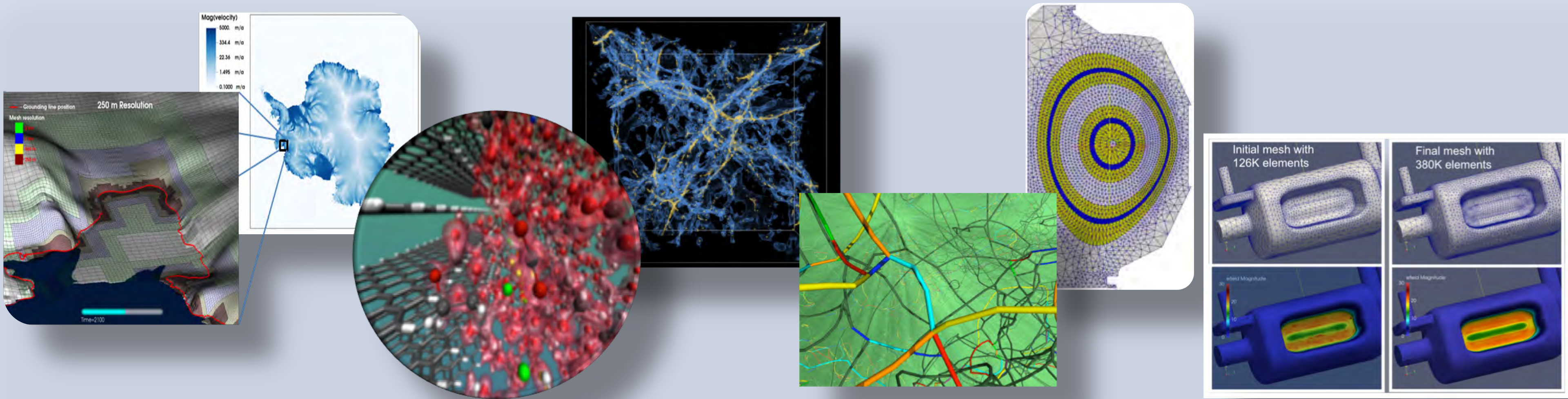
FASTMath brings together an exceptional team of researchers and software library capabilities

Our team comprises over 50 researchers from 5 national laboratories and 5 universities

Our software has 100s of person years of development behind it

For more information contact: Lori Diachin, LLNL
diachin2@llnl.gov

The FASTMath team has a proven record of advancing application simulation codes



Next Generation Application Codes

- Created unique DOE capabilities in ice sheet modeling
- First ever, self consistent solution of continuum gyrokinetic system in edge plasmas
- Unprecedented resolution for Nyx cosmology code

Faster Time to Solution

- New eigensolvers 2X faster for quantum chemistry software
- Parallel PEXSI software enabled electronic structure calculations with 10,000 atoms (compared to 1000's)
- Accelerated nonlinear solver enabled largest dislocation dynamics simulation with ParaDiS

More Robust Simulations

- Dramatically decreased time to generate meshes for fusion tokamak codes
- Adaptive mesh refinement and discretizations to resolve ELM disruptions in tokamaks
- Order of magnitude improvement in accuracy of integral calculations in material chemistry

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For more information contact: Lori Diachin, LLNL
diachin2@llnl.gov

FASTMATH

FASTMath is actively engaged with 19 SciDAC-4 application partnerships

BER (5)

- Structured grid AMR
- Unstructured grid AMR
- Time integration
- Linear/Nonlinear solvers, Preconditioners
- Optimization
- Verification / UQ

FES (5)

- Unstructured meshes
- Discretization technologies
- Iterative Linear solvers
- UQ

HEP (3)

- Direct solvers
- Structured Grid AMR
- Optimization
- Sensitivity Analysis
- Inference and machine learning

NP (2)

- Structured grid AMR
- Eigenvalue problems
- Inference and Machine Learning

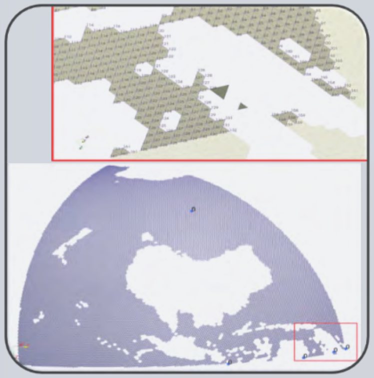
BES (2)

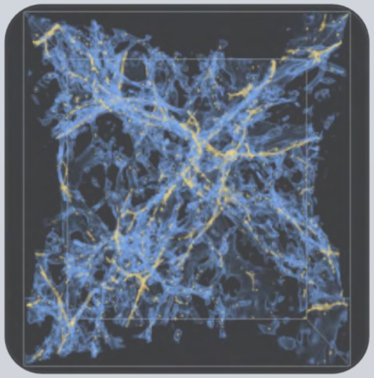
- Nonlinear and tensor eigenvalue problems
- Linear solvers and Preconditioners

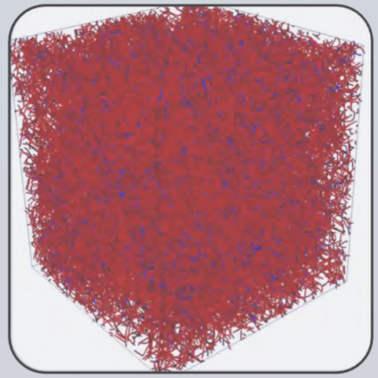
NE (1)

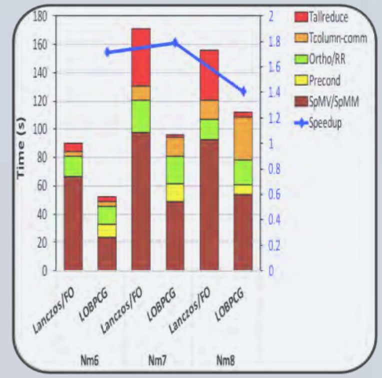
- UQ

Math-CS collaborations led to significant advances in SciDAC-3 application sciences









Increased accuracy of MPAS Ocean modeling system through improved scaling and improved partitioning algorithms

Development of highly-scalable, many core-aware multigrid solver increased ability of cosmologies to simulated evolution and fate of the universe (HPGMG in BoxLib)

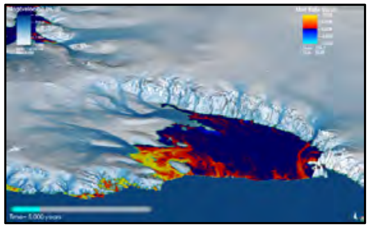
New nonlinear solver and evaluation of OpenMP performance enabled largest dislocation dynamics simulation using ParaDiS

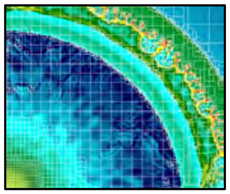
Improved efficiency of eigensystem solution reduced time to solution in large, sparse ab initio calculations in nuclear structure

FASTMath and RAPIDS will actively collaborate to continue to improve math libraries and application experience

- **Performance improvements to math library software**
  - Improved scaling (identify performance bottlenecks, find ‘performance bugs’, eliminate unnecessary communication)
  - Improved on-node performance (programming models, memory)
- **Using performance models to improve foundational understanding of algorithms**
- **Advanced visualization tools for FASTMath tools (e.g., AMR)**
- **In situ visualization tools used in unstructured mesh simulation workflow**
- **Use of CS abstractions to improve or accelerate application development**
  - Domain Specific Language compilers/tools
  - Leverage abstractions developed by RAPIDS for I/O to unify application experience

FASTMath is focused on eight core technology areas





Structured Mesh Spatial Discretization

Data Analytics

Unstructured Mesh Spatial Discretization

Synergistic activities link the eight areas together

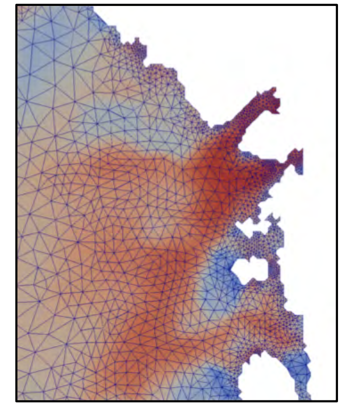
Uncertainty Quantification

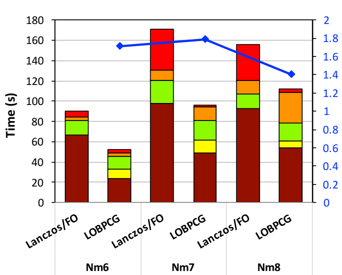
Time Integrators

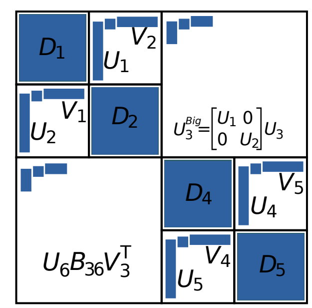
Numerical Optimization

Solution of Linear Systems

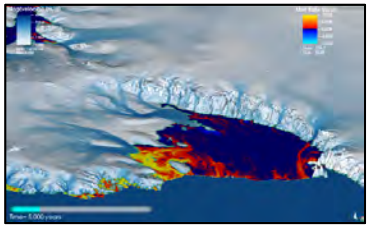
Solution of Eigenvalue Problems

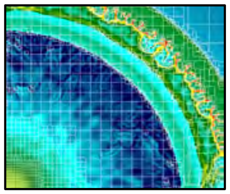






Eight core technology areas: Structured Mesh





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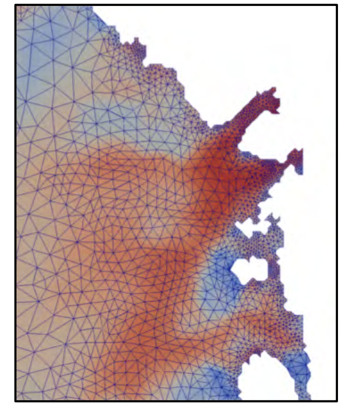
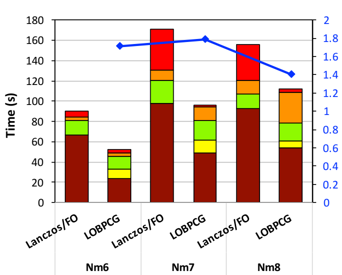
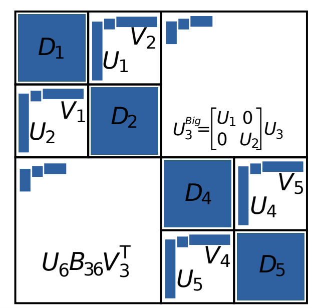




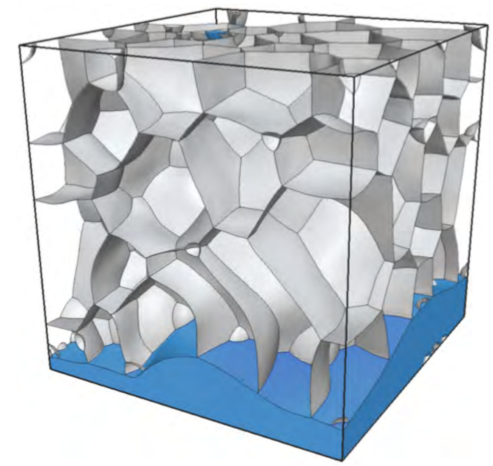


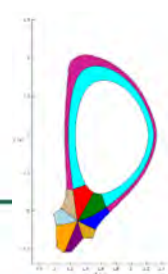
For more information contact: Ann Almgren (LBNL), asalmgren@lbl.gov

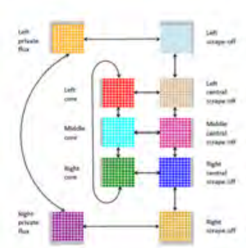
FASTMath Structured Mesh Activities

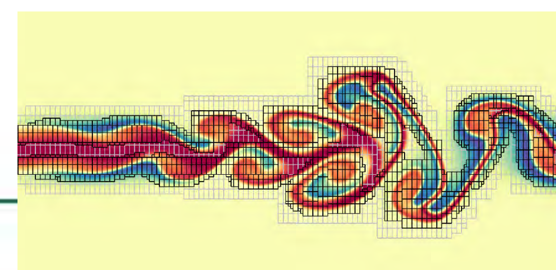
FASTMath supports several structured mesh frameworks with a wide range of capabilities.   Features include support for

- Adaptive Mesh Refinement (AMR)
- Higher-order interior spatial discretizations
- Higher-order time-stepping
- Higher-order tools for interface dynamics
- Particle dynamics and particle-mesh operations
- Mapped multi-block domains
- Dynamic load balancing
- Interoperability with other solvers, e.g. those in SUNDIALS, PETSc, hypre



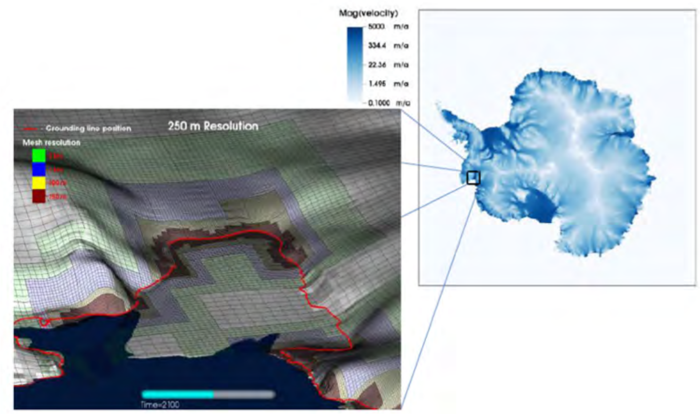






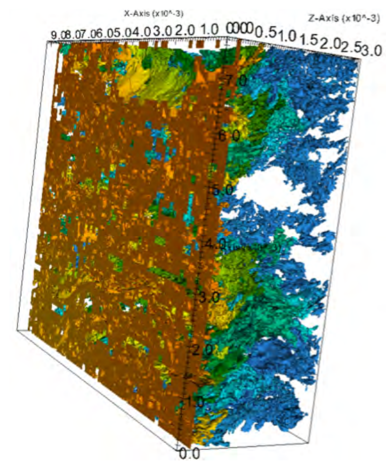
Structured Mesh Application Areas

- FASTMath structured grid capabilities are used in numerous DOE projects:



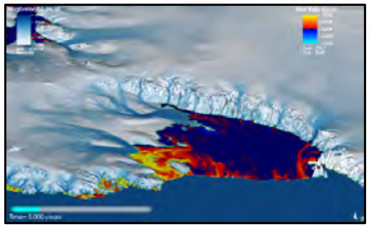
- **SciDAC-4**:
  - ComPASS (PIC with AMR)
  - TEAMS (astrophysics)
  - ProSPect (BISICLES ice sheet model)

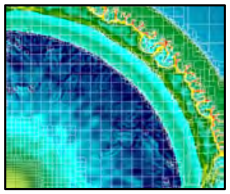
- **HPC4Mfg**
  - 3D printing
  - industrial spray painting
  - combustion with electric fields



- **ECP** – accelerator modeling, astrophysics, combustion,
- cosmology, multiphase flow, subsurface

Eight core technology areas: Unstructured Meshes





Structured Mesh Spatial Discretization

Unstructured Mesh Spatial Discretization

Data Analytics

Time Integrators

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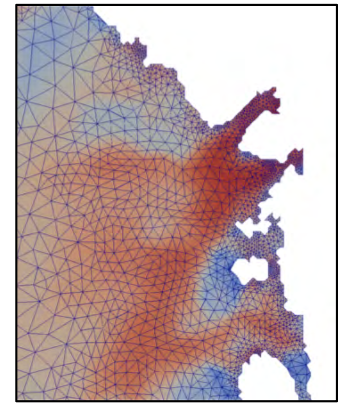
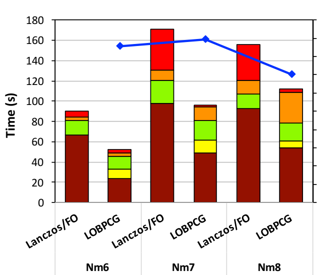
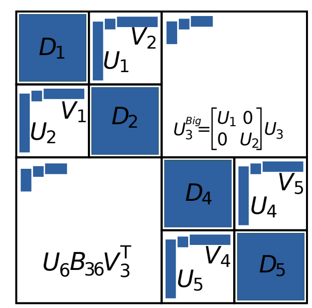
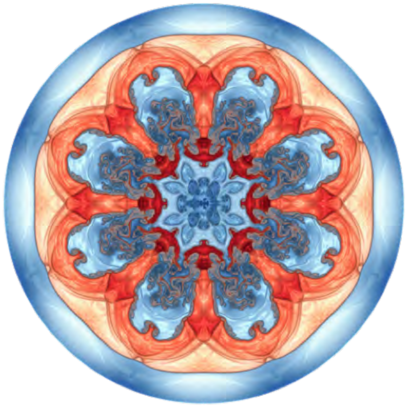




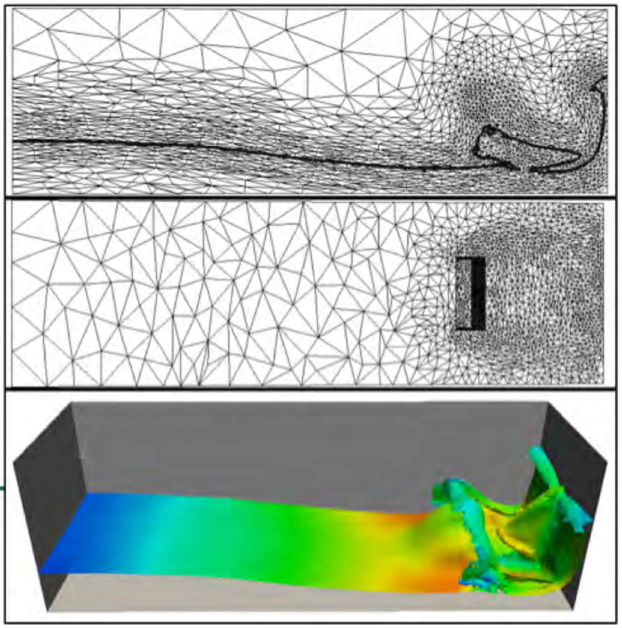


FASTMath Unstructured Mesh Development Areas

FASTMath is providing application developers with tools and methods so they can take direct advantage of the advantages of unstructured mesh technologies.

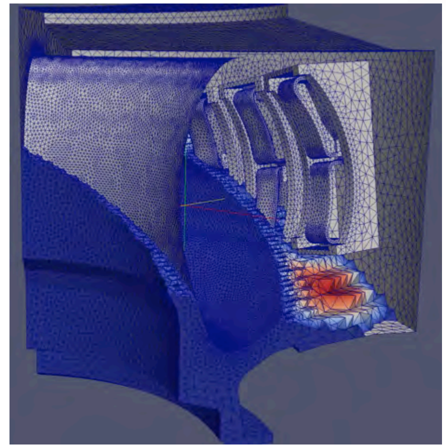


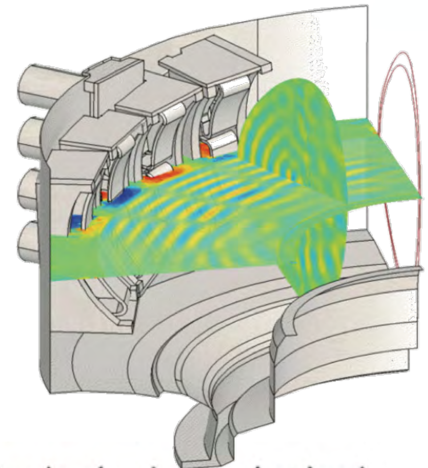
- Unstructured Mesh Analysis Codes
- Unstructured Mesh Adaptation
- Performant Unstructured Meshes
- Dynamic Load Balancing and Task Mapping for Extreme Scale Applications
- Unstructured meshes for:
  - PIC methods
  - Management of UQ processes
  - In situ visualization and data analytic

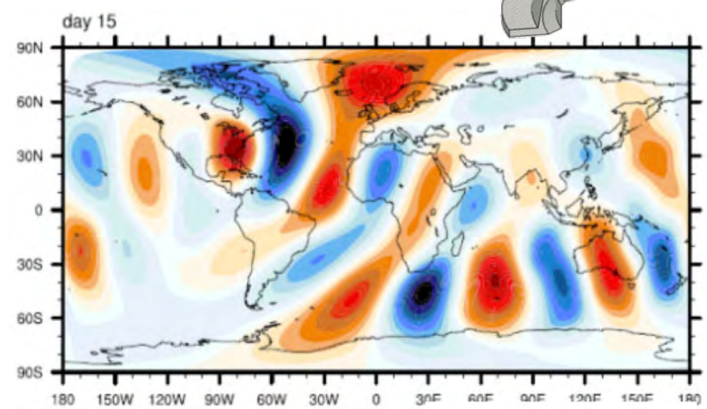


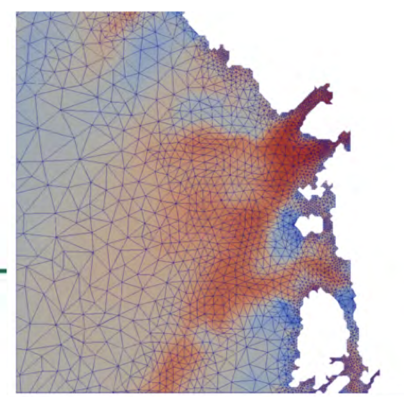
Subset of Current Unstructured Mesh Application Areas

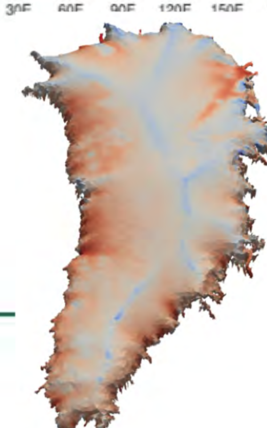
- Analysis of RF waves in tomamak fusion reactors
  - MFEM high-order finite elements
  - PUMI geometry and mesh control
- Atmospheric Modeling
  - Zoltan2's task placement to reduce communications in HOMME's simulations
- Modeling ice sheet melting
  - Core simulation in for sea level predictions
  - FELIX analysis code
  - Omega_h mesh adaptation
- Unstructured mesh methods for 4 fusion SciDACS



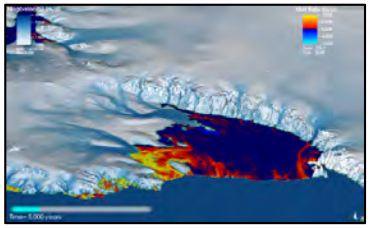


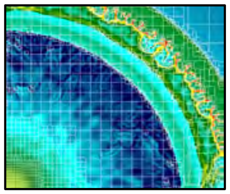






Eight core technology areas: Time Integrators





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Synergistic activities link the eight areas together

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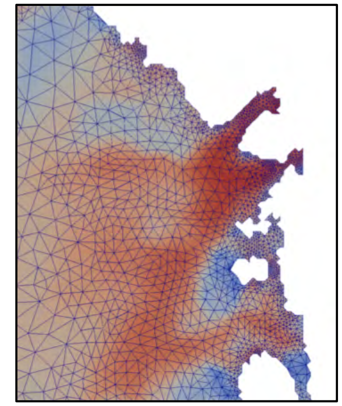
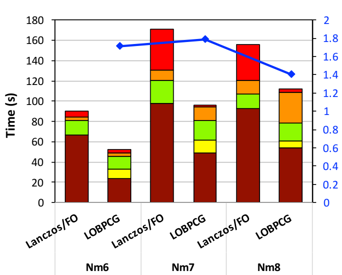
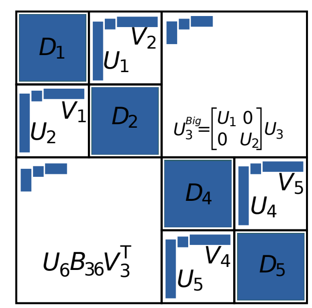






For more information contact: Carol Woodward (LLNL), cswoodward@llnl.gov

FASTMath activities support several time integration methodologies and software

FASTMath supports:

- Multistep and multistage adaptive time stepping software for ordinary differential equations and differential algebraic equations
- Spectral deferred correction methods and software that include iterative and parallel methods for the time domain
- Adjoint integration methods and software (for discrete and continuous adjoints) for application to optimization contexts

Planned activities:

- Multirate methods in SUNDIALS
- Parallel-in-time methods in SUNDIALS
- High order SDC methods in AMReX
- Multilevel and implicit/explicit SDC methods in AMReX
- Second-order discrete adjoint capabilities in PETSc

FASTMath time integration methods are delivered through software and personnel expertise

Software

- SUNDIALS (https://computation.llnl.gov/projects/sundials)
- PETSc (www.mcs.anl.gov/petsc)
- SDC in AMReX (amrex-codes.github.io)
- Libpfasst (pfasst.lbl.gov)

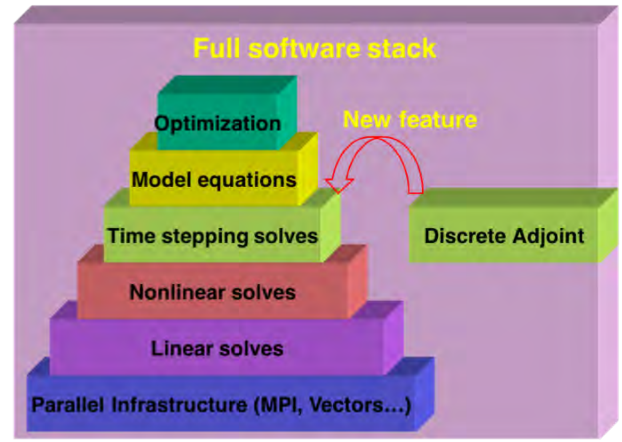
Personnel:

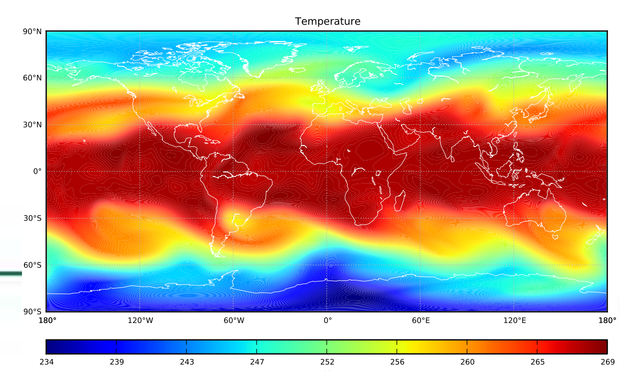
- LLNL: Woodward, Gardner, Loffeld
- LBNL: Minion
- ANL: Zhang, Smith
- SMU: Reynolds

FASTMath activities target innovation in methods and software that will impact applications

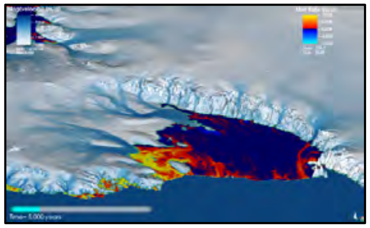
DOE applications targeted:

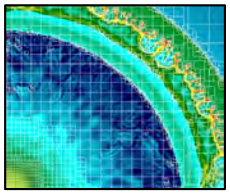
- **Climate**
  - atmospheric dynamics and physics
  - ice sheets
- **Combustion**
- **Power grid**
- **Cosmology**
- **Subsurface flow**
- **Additive manufacturing**

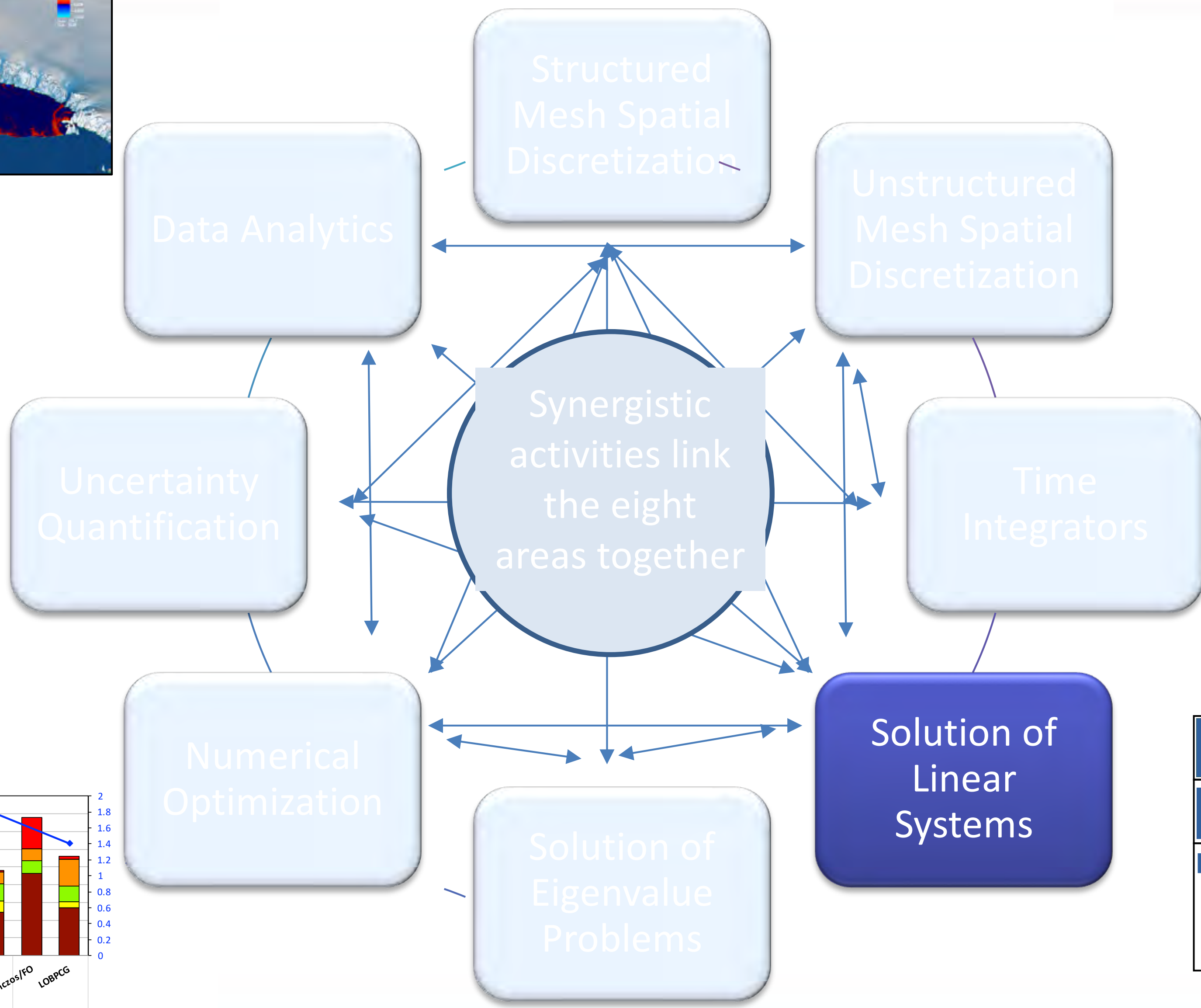


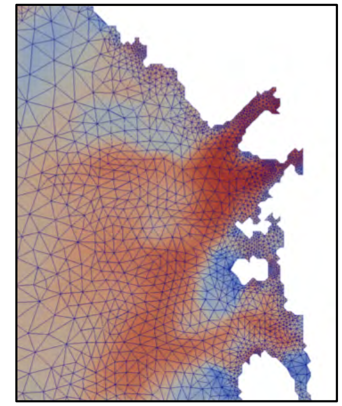


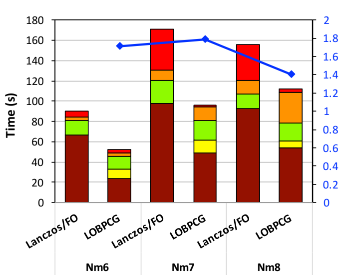
Eight core technology areas: Linear Systems

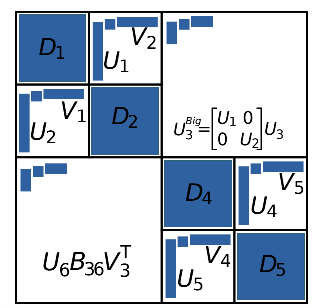








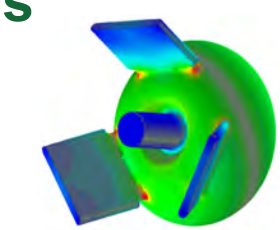




For more information contact: Ulrike Yang (LLNL), yang11@llnl.gov

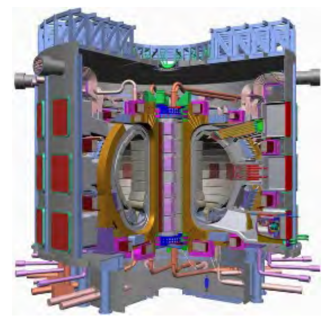
FASTMath Linear Solvers Impact Many Applications

- **FASTMath provides a variety of linear solvers to address different needs of DOE applications,
such as climate, astrophysics, nuclear physics, fusion, subsurface flow, additive manufacturing, power grid**

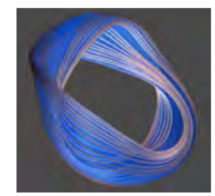


Electro-magnetics

- **Tokamak Transient Simulations**

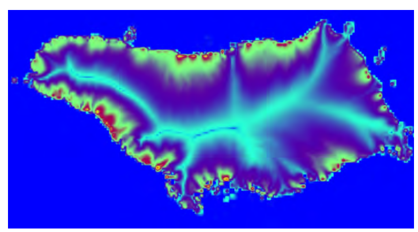


ITER Tokamak

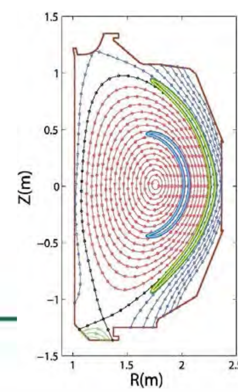


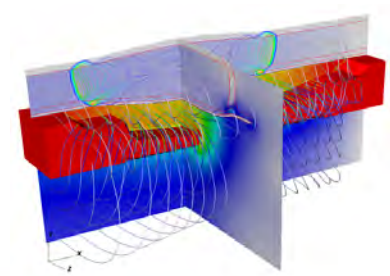
Magneto-hydrodynamics

- **Land ice simulations**



- **Simulation of Energetic Particles in Burning Plasmas**

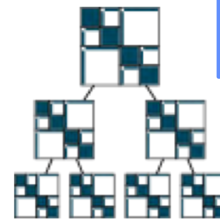


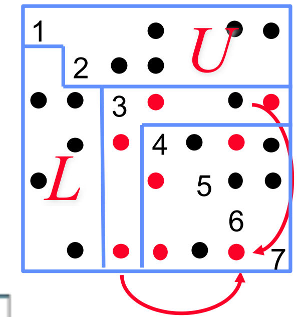


Magnetic flux compression generator simulation enabled by MG smoother research

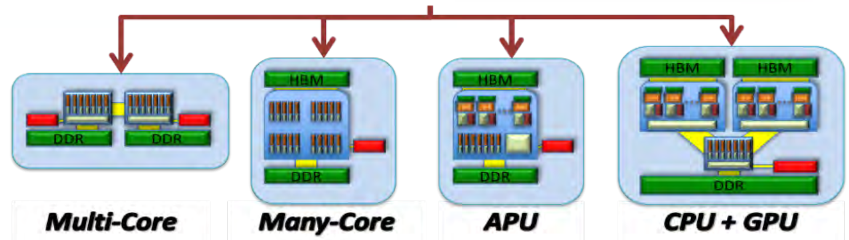
FASTMath Linear Solvers Software

- SuperLU – LU factorizations
- symPACK – symmetric positive definite matrices
- STRUMPACK – hierarchical basis preconditioners
- PDSLin – parallel domain decomposition Schur complement based linear solver
- Local discrete convolution methods (LDCMs) for constant coefficient PDEs
- ShyLU (Trilinos) - domain decomposition and node level solvers, including BDDC and GDSW preconditioners, Multithreaded LU, Cholesky, and triangular solvers



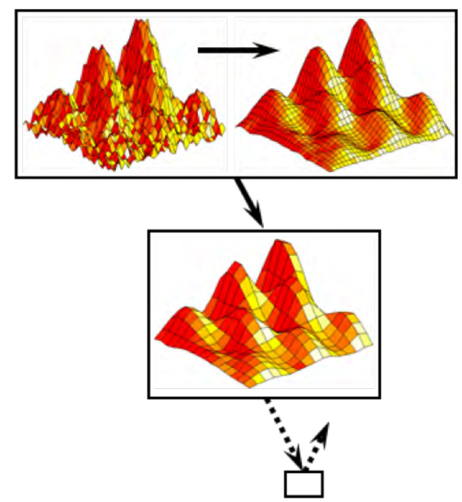


FASTMath Linear Solvers Software

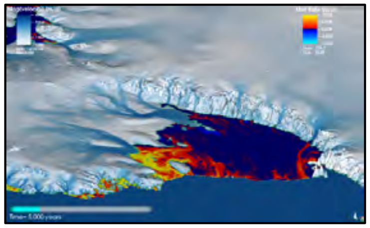


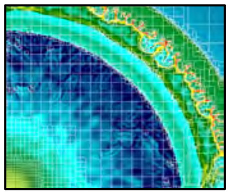
- **KokkosKernels:**
  basic linear algebra kernels
- **Highly scalable multigrid solvers and preconditioners with different flavors**
  - Hypre: structured and unstructured multigrid solvers, conceptual interfaces
  - MueLU (Trilinos): smoothed aggregation multigrid solvers
  - GAMG (PETSc): geometric, algebraic, hybrid options
- **Krylov solvers (PETSc, hypre, …)**

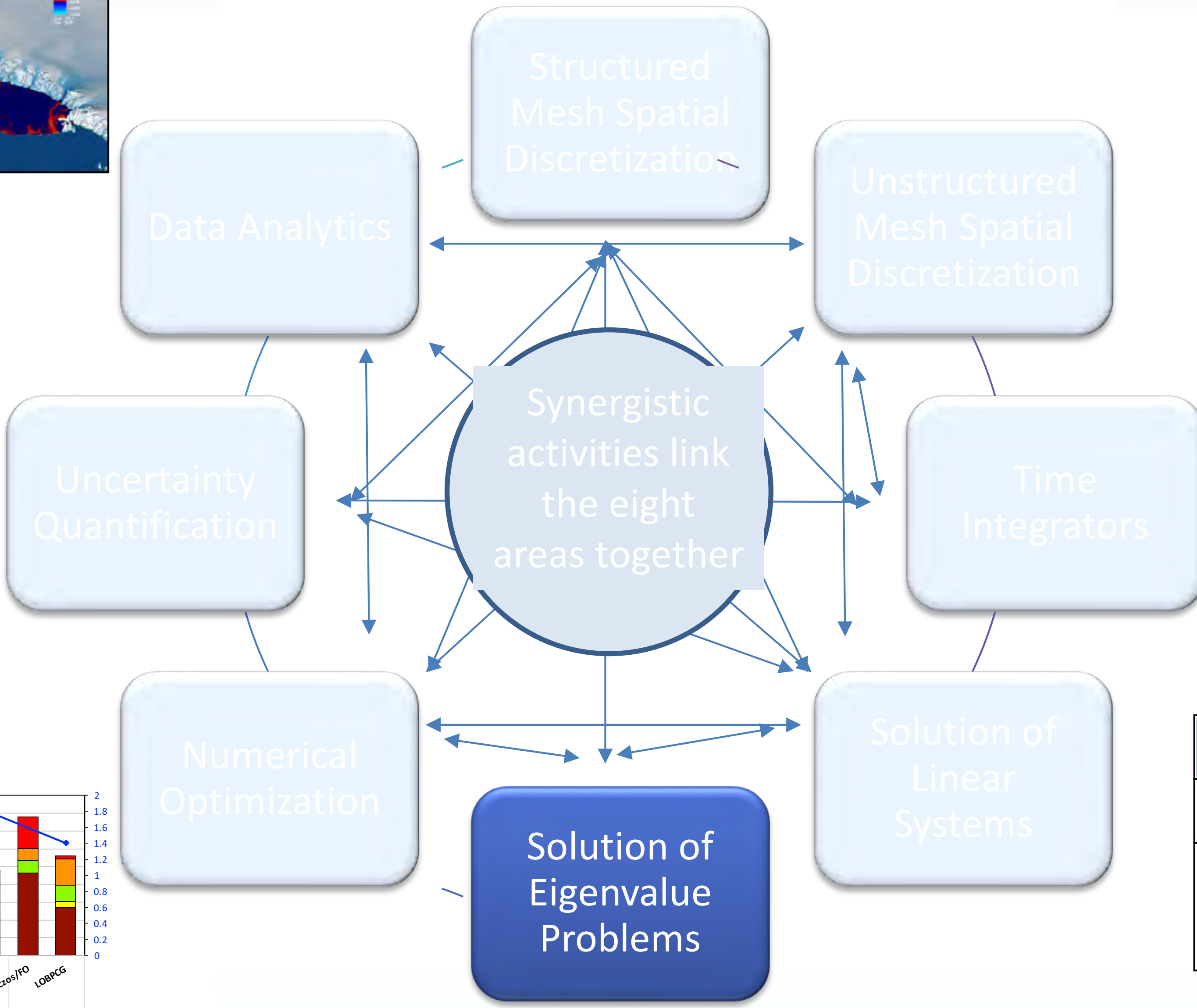
hypre high performance preconditioners

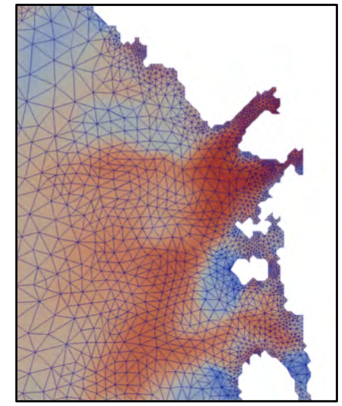


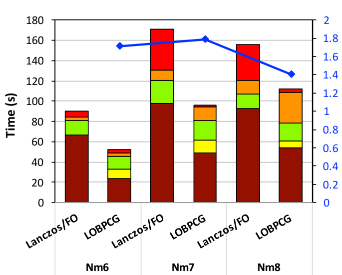
Eight core technology areas: Eigenvalue Problems

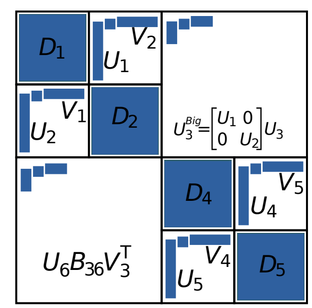








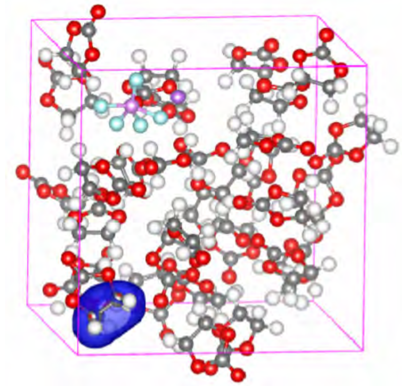




For more information contact: Chao Yang (LBNL), cyang@lbl.gov

FASTMath Eigensolver Activities

FASTMath supports numerical solutions of large-scale eigenvalue problems of a variety types.



- **Hermitian eigenvalue problems**
- **Non-Hermitian eigenvalue problems**
- **Nonlinear eigenvalue problems with eigenvector nonlinearity**

$$H(X)X = X\Lambda$$

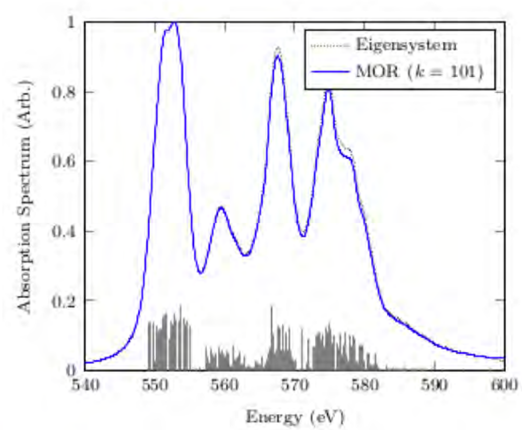
- **Nonlinear eigenvalue problems with eigenvalue nonlinearity**

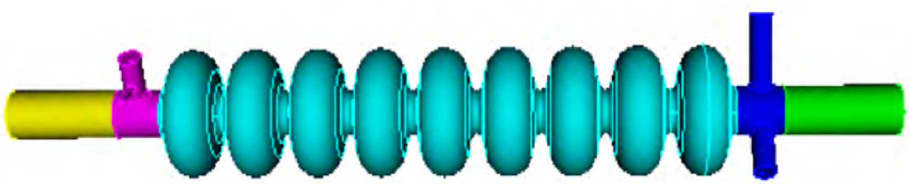
$$T(\lambda)x = 0$$

- **Eigenvalue problems with Tensor structures**

$$H = \sum_{i=1}^{L} I \otimes \cdots \otimes A_i \otimes A_{i+1} \otimes I \cdots$$

- **Linear response eigenvalue problem**



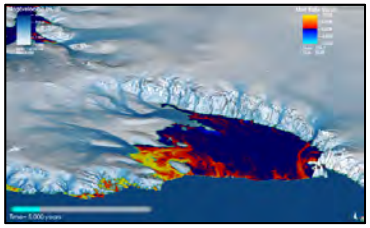


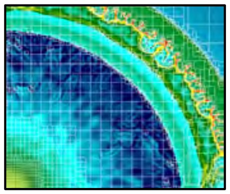
Eigensolver Application areas

FASTMath eigensolvers are used in several DOE applications

- **SciDAC-4**
  - Catalysis (Kohn-Sham DFT nonlinear eigenvalue problem)
  - Topological materials (Tensor eigenvalue problem)
  - Nuclei structure (Many-body eigenvalue problem)
- **Computational Materials Center (linear response eigenvalue problem, spectroscopy)**
- **Computational Chemistry Center (linear response eigenvalue problem, spectroscopy)**
- **ECP (NWChem)**

Eight core technology areas: Numerical Optimization





Structured Mesh Spatial Discretization

Data Analytics

Unstructured Mesh Spatial Discretization

Synergistic activities link the eight areas together

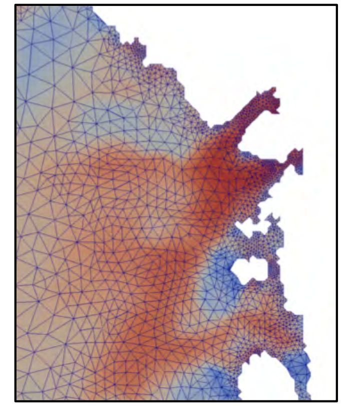
Uncertainty Quantification

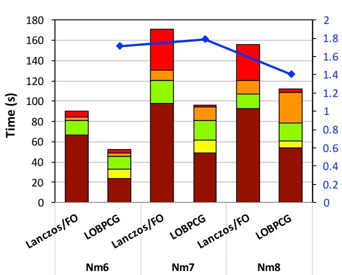
Time Integrators

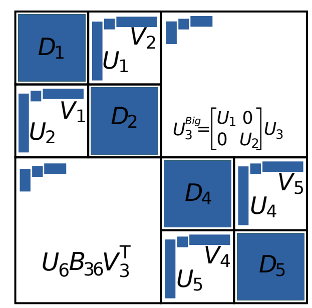
Numerical Optimization

Solution of Linear Systems

Solution of Eigenvalue Problems







For more information contact: Todd Munson (ANL), tmunson@mcs.anl.gov

Numerical Optimization Activities

Develop methods for numerical optimization problems with constraints and for sensitivity analysis using adjoint capabilities.

Dynamic Optimization

- Deliver new capabilities for problems with PDE constraints that include:
  - Dynamics and controls
  - State and design constraints
  - Discrete variables
  - Multiple objectives
- Support a range of derivative requirements

Sensitivity Analysis

- Develop iterative sampling methods that employ sensitivity analysis and surrogate models to determine the most important parameters
- Explore multilevel approach that uses a low-fidelity model to predict parameter sensitivities

Adjoints

- Develop advanced adjoint and forward sensitivity capabilities to provide derivative information
- Provide methods for computing the action of second-order adjoints
- Support calculations involving several quantities of interest

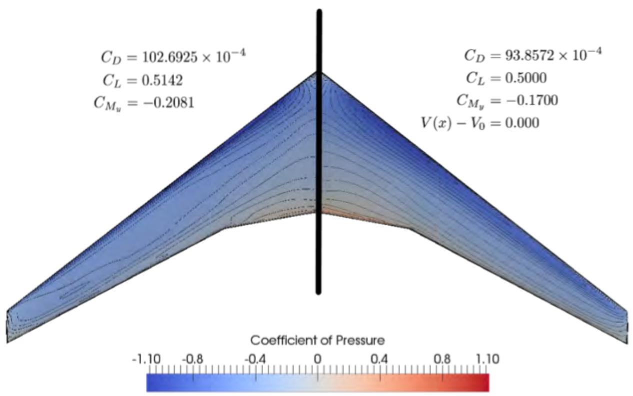
For more information: Todd Munson (tmunson@mcs.anl.gov)

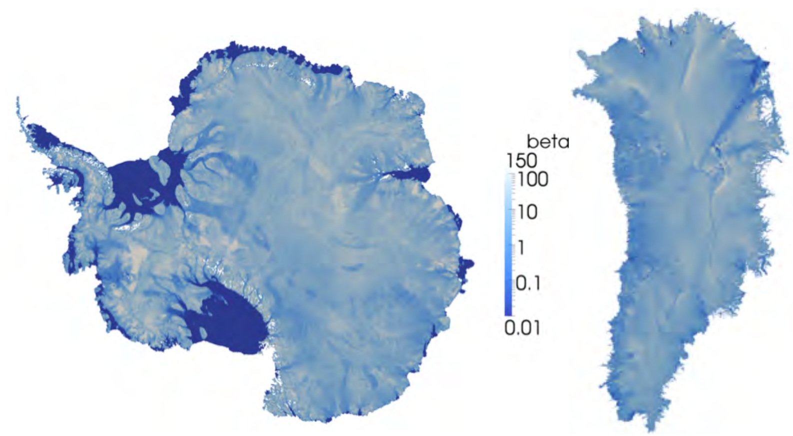
Numerical Optimization Overview

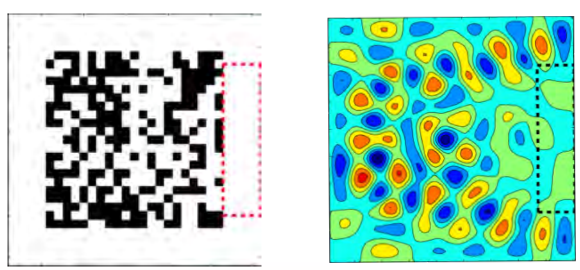
$$
\begin{aligned}
\underset{\mathbf{x},\mathbf{u}}{\text{minimize}} \quad & \mathcal{J}(\mathbf{x},\mathbf{u}) \\
\text{subject to} \quad & \mathbf{C}(\mathbf{x},\mathbf{u}) \leq \mathbf{0} \\
& \mathbf{R}(\mathbf{x},\mathbf{u}) = \mathbf{0}
\end{aligned}
$$

$\mathbf{x}$: Design variables

$\mathbf{u}$: State variables





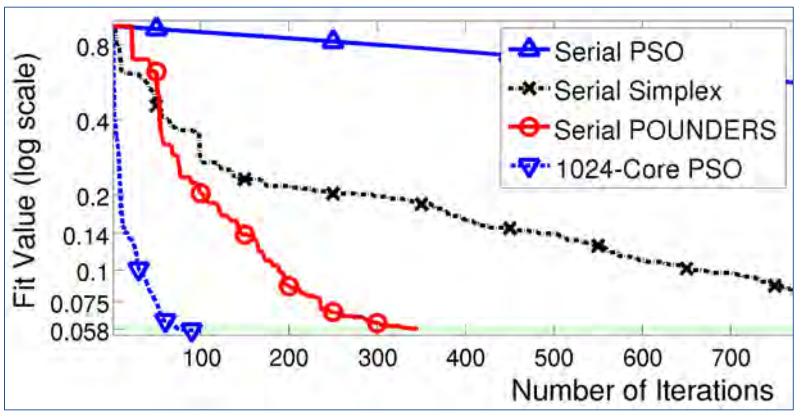


Left: aerodynamic shape optimization
Middle: design of electromagnetic scatterer
Right: ice sheet inversion

Numerical Optimization Software and Applications

Software Development

- **APOSMM, MATSuMoTo, ORBIT, POUNDERS**
  - Derivative-free optimization
- **MINOTAUR**
  - Mixed-integer nonlinear optimization
- **TAO, ROL**
  - PDE-constrained optimization

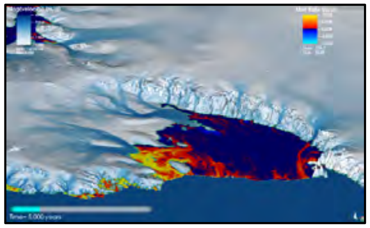


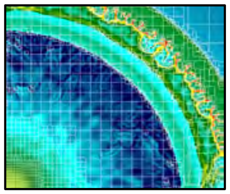
Exploiting structure in particle accelerator calibration

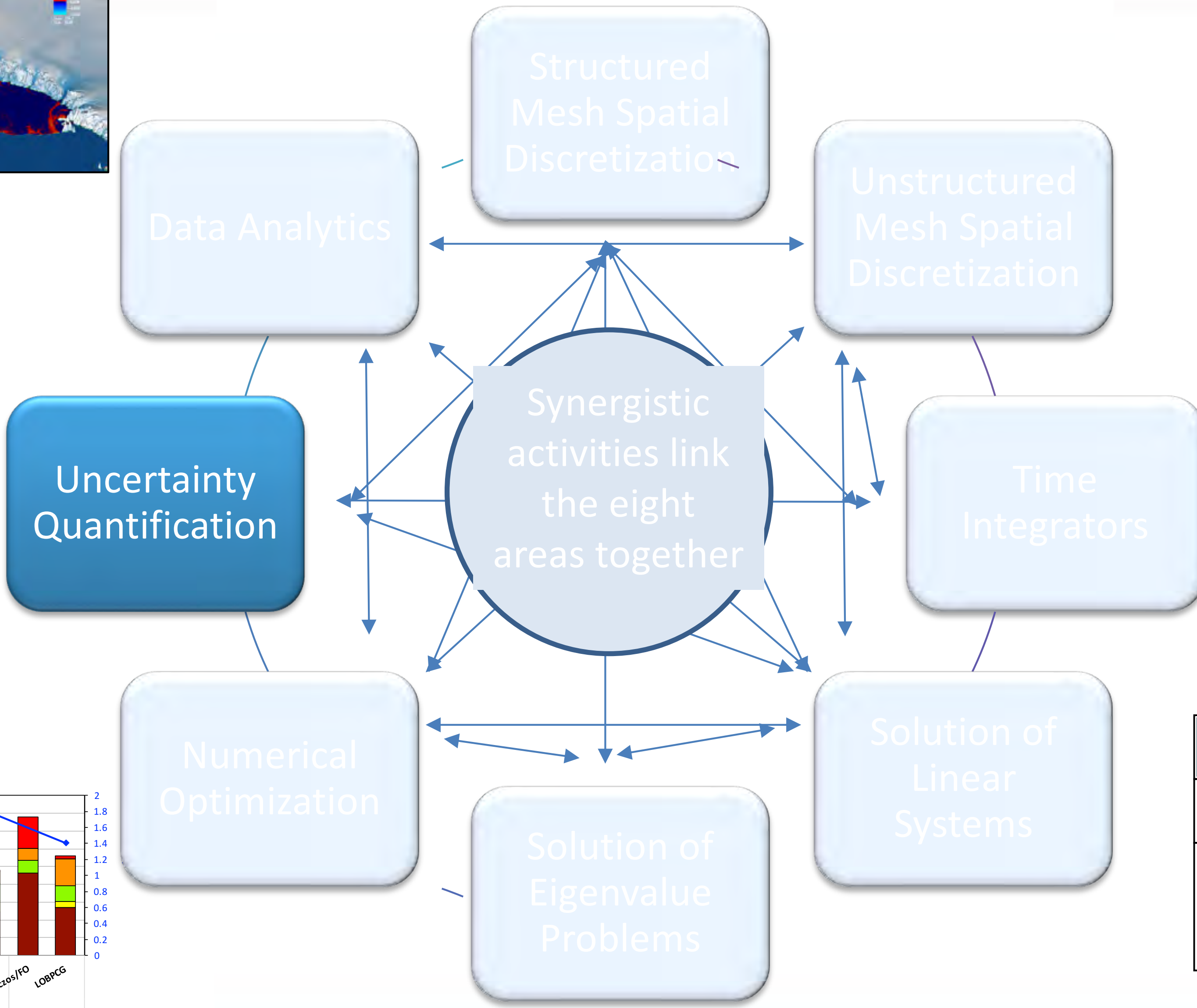
Applications

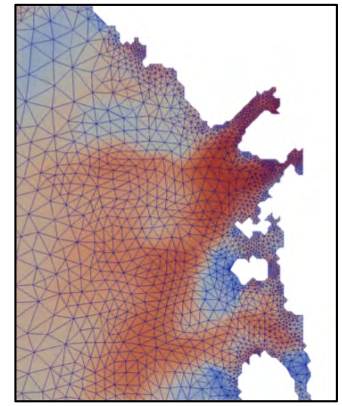
- **NP: Nuclear Computational Low Energy Initiative (NUCLEI)**
  - Calibration and optimization of energy density functionals
- **HEP: Community Project for Accelerator Science & Simulation (ComPASS4)**
  - Particle accelerator design
- **HEP: Accelerating HEP Science: Inference and Machine Learning at Extreme Scales**
  - Multi-fidelity optimization and Bayesian parameter estimation
- ***HEP:* Data Analytics on HPC**
  - Least-squares problems with integer variables and sensitivity analysis
- ***BER:* Probabilistic Sea-Level Projections from Ice Sheet and Earth System**
  - Transient PDE-constrained optimization

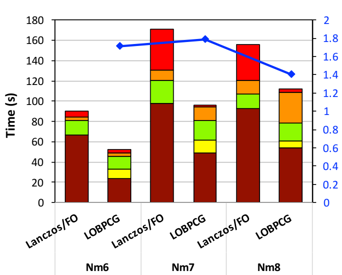
Eight core technology areas: Uncertainty Quantification

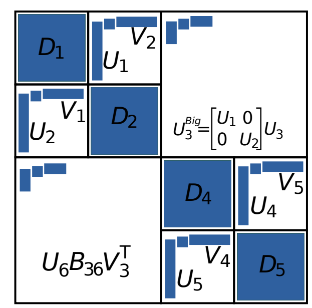








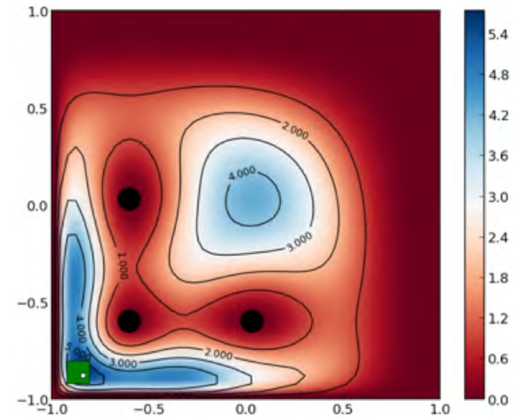


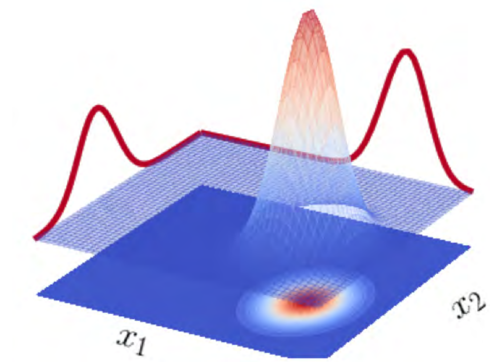


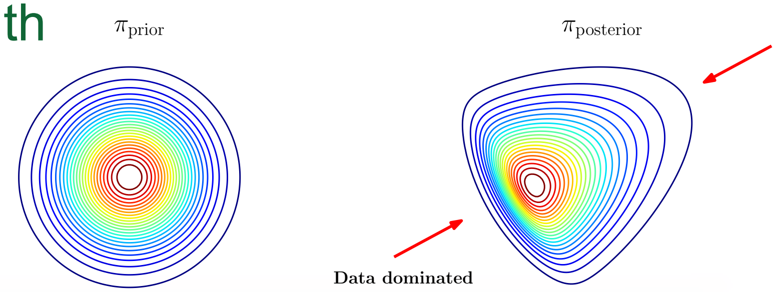
For more information contact: Habib Najm (SNL), hnnajm@sandia.gov

Uncertainty Quantification – Ongoing work

- **High dimensional function representations**
  - Polynomial regression, compressive sensing
  - Low rank tensors, basis adaptation, manifolds
- **Multilevel Multifidelity (MLMF)**
  - Monte Carlo, PCE via sparse/low-rank
  - Resource allocation across model form and discretization level hierarchies
- **Bayesian inference**
  - Data-informed subspace, model error
- **Optimization under uncertainty (OUU)**
  - Recursive trust region model management with deep hierarchies
  - Reliability-based OUU based on efficient estimation of rare events

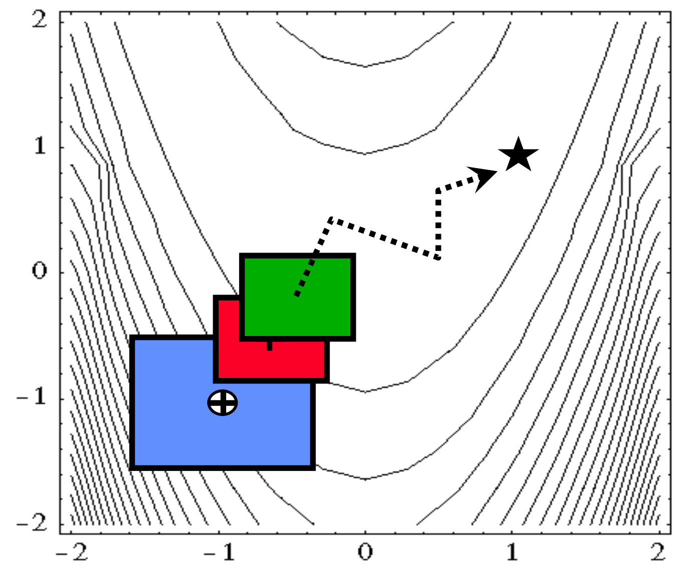


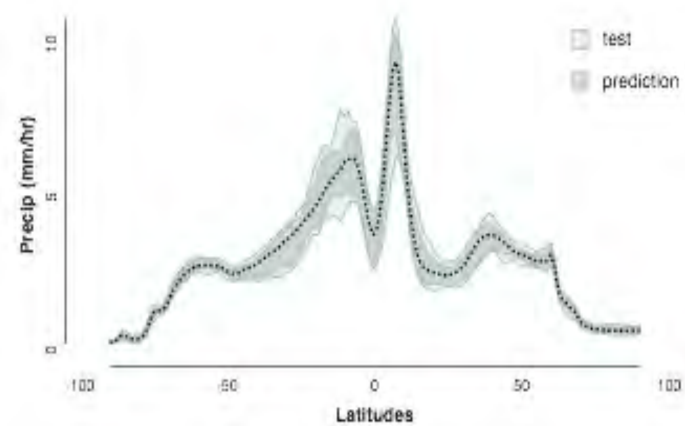




Description of the UQ software tools

- **DAKOTA**
  - Uncertainty quantification and Optimization
  - Open source (GNU LGPL)
  - dakota.sandia.gov
- **UQ Toolkit – UQTk**
  - Uncertainty quantification
  - Open source (GNU LGPL)
  - www.sandia.gov/UQToolkit





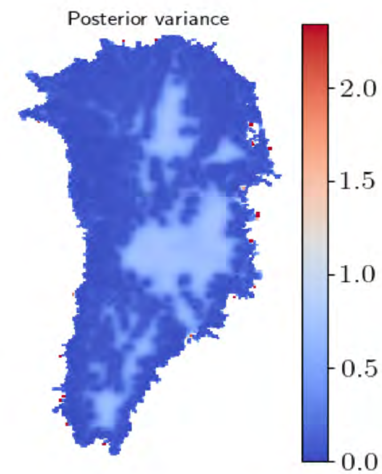
UQTk

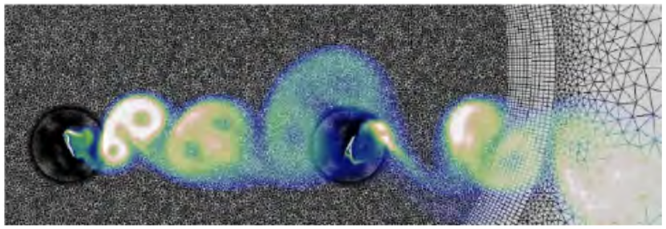
DAKOTA

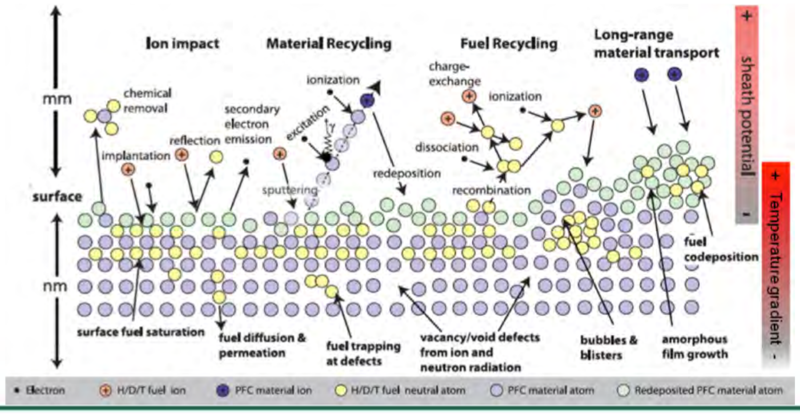
Explore and predict with confidence

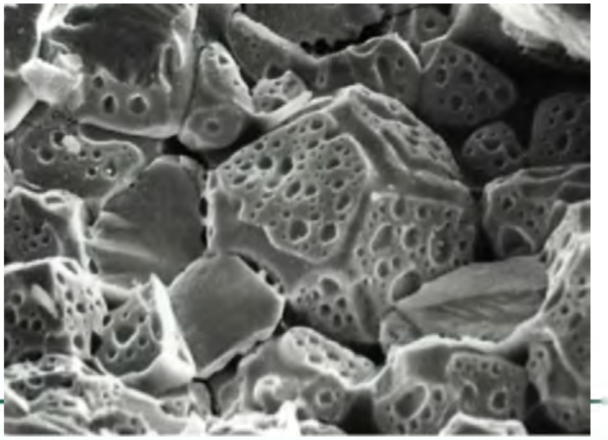
UQ Application interactions

- Ice sheet and earth system modeling
- Tokamak disruption simulation
- Exascale wind flow modeling
- E3SM climate modeling
- Sensor networks for climate modeling
- Fusion plasma surface interactions
- Fission gas in nuclear fuel

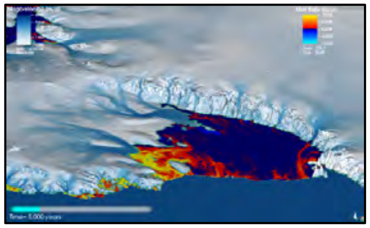


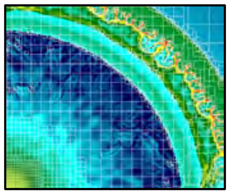


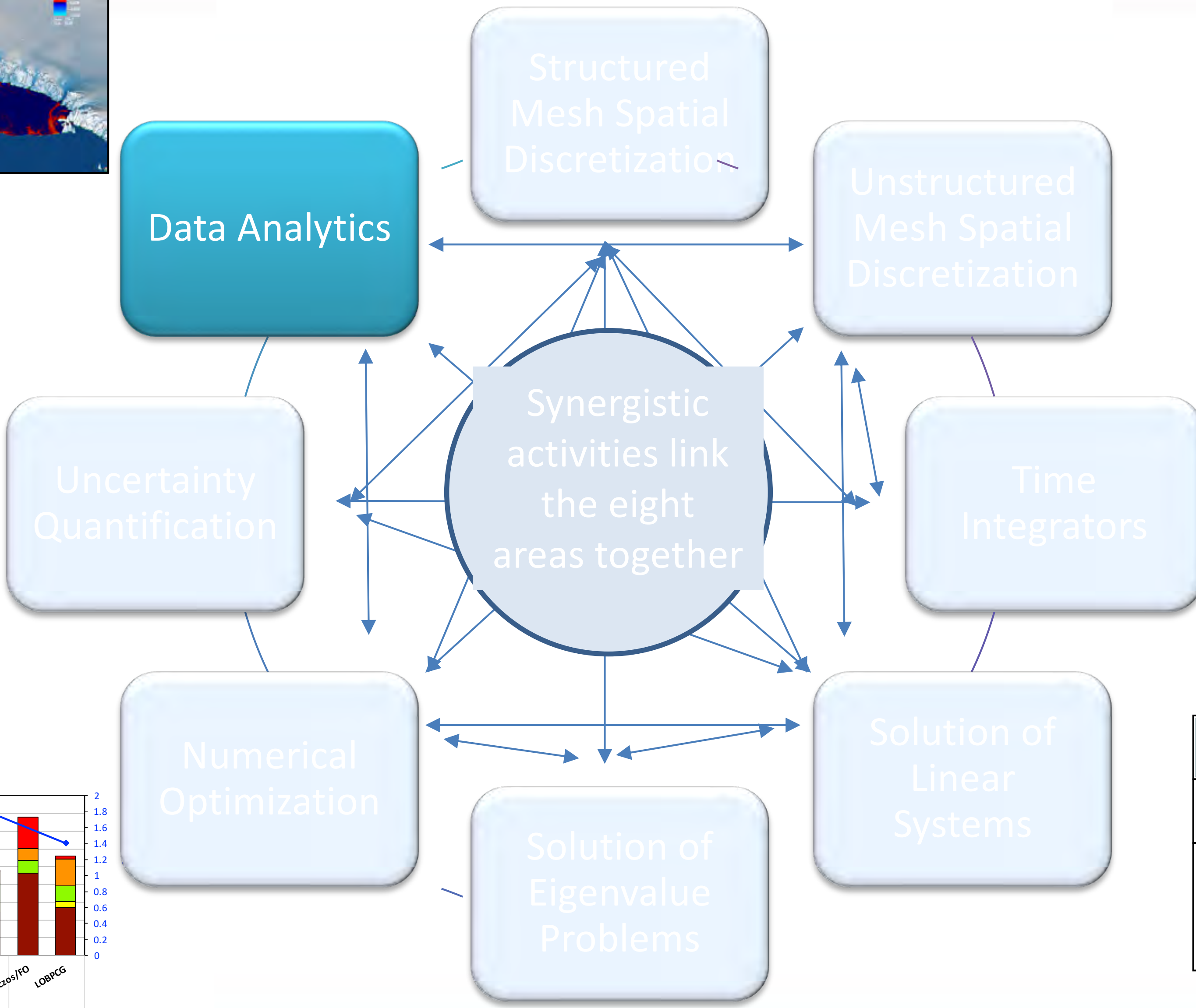


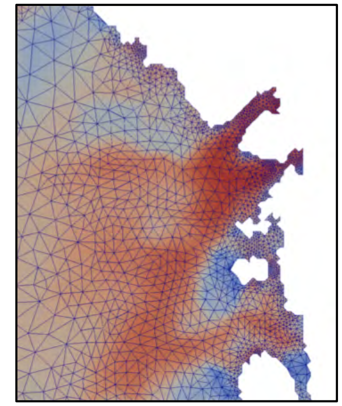


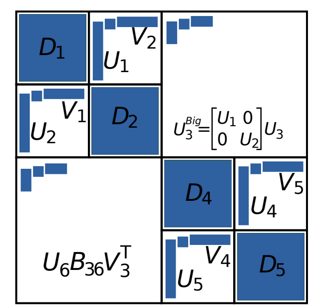
Eight core technology areas: Data Analytics

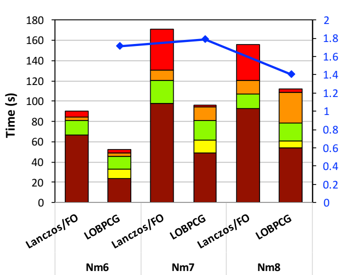






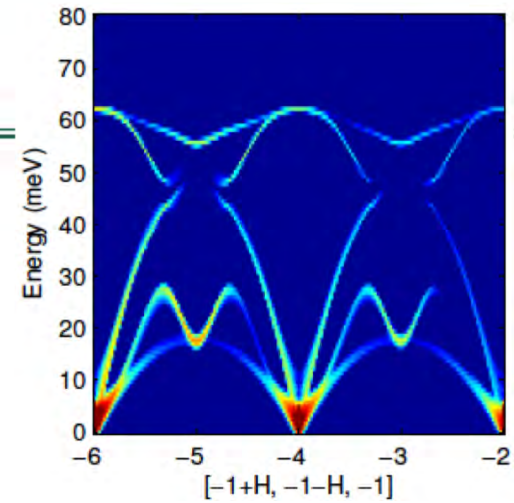






For more information contact: Rich Archibald (ORNL), archibaldrk@ornl.gov

Data Analytics



- **Goal: Sparse functional representation of data, to enable faster IO and analysis of big datasets**
- **Software tools: Tasmanian, PUMI, TAO**
- **FASTMath Tasks**

Sparse IO of Big Data

- Advanced sampling techniques for distributed data
- Research adaptive methods for sparse representation
- Build accurate uncertainty estimates for sparse representations of data

Fast Estimation & Evaluation

- Develop and design high order regularizes that optimize functional representations of data
- Surrogate models that accelerate estimation and evaluation of sparse data approximation

Streaming Data Ranking

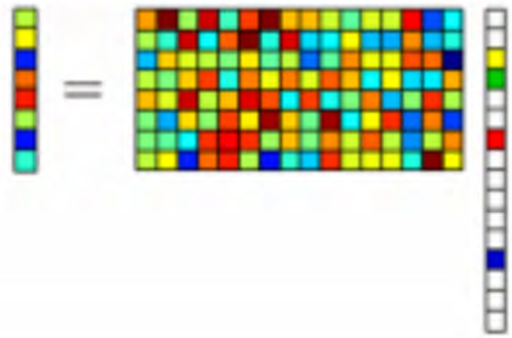
- Algorithms that maximize information transfer
- Ordered sparse functional representations of data
- Parallel methods for streaming distributed datasets

- **For more information**: Rick Archibald (ArchibaldRK@ornl.gov), Clayton Webster (ORNL), & Hoang Tran (ORNL)

Data Analytics: Technical description of technology

- **We reconstruct data $c \in \mathbb{R}^{N\times l}$ from measurements $u \in \mathbb{R}^{m\times l}$ and $A \in \mathbb{R}^{m\times N}$:**

$$u \approx Ac$$



  - Limited number of measurements: $m \ll N$.
  - The data are sparse.
  - $l = 1$: reconstructing a single dataset.
    $l > 1$: simultaneously reconstructing multiple datasets.

- Recovery via regularizations enforcing sparsity:

$$c = \text{argmin}\, R(z) \quad \text{subject to} \quad u \approx Az$$

Standard CS: $R(z) = \|z\|_1$.

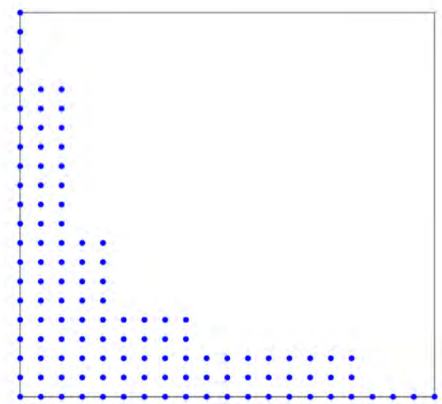
Structures of the sparsity can be exploited:

- Downward closed and tree structures: $R(z) = \|z\|_{\omega,1}$.
- Joint sparsity: $R(z) = \|z\|_{2,1}$.

Data Analytics: Technical description of technology

- **Data from UQ and imaging applications often possess downward closed and tree structure.**
- Weighted l_1 minimization with a specific choice of weight:

$$R(z) = \|z\|_{\omega,1} \text{ with } \omega_j = \max |A_{:,j}|$$



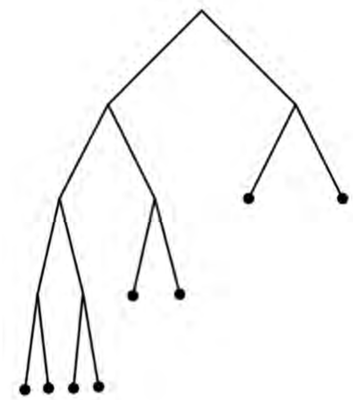
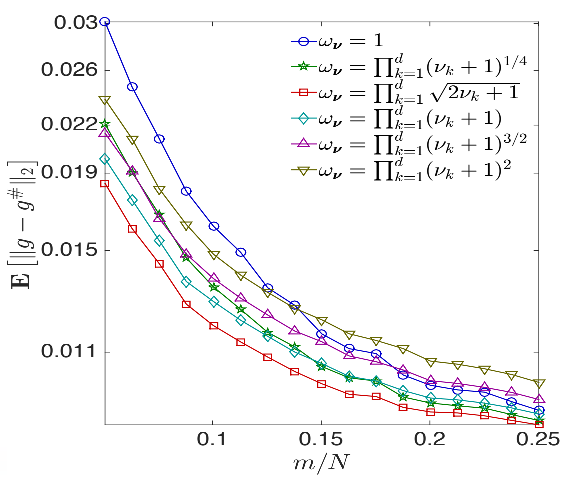


Figure: *A comparison of weighted l_1 minimization with different choices of weights*

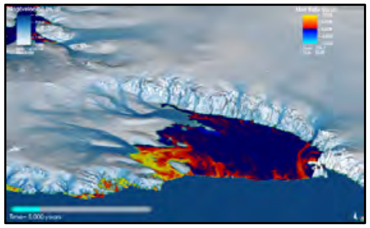


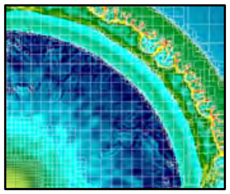
Certified reduction in complexity:

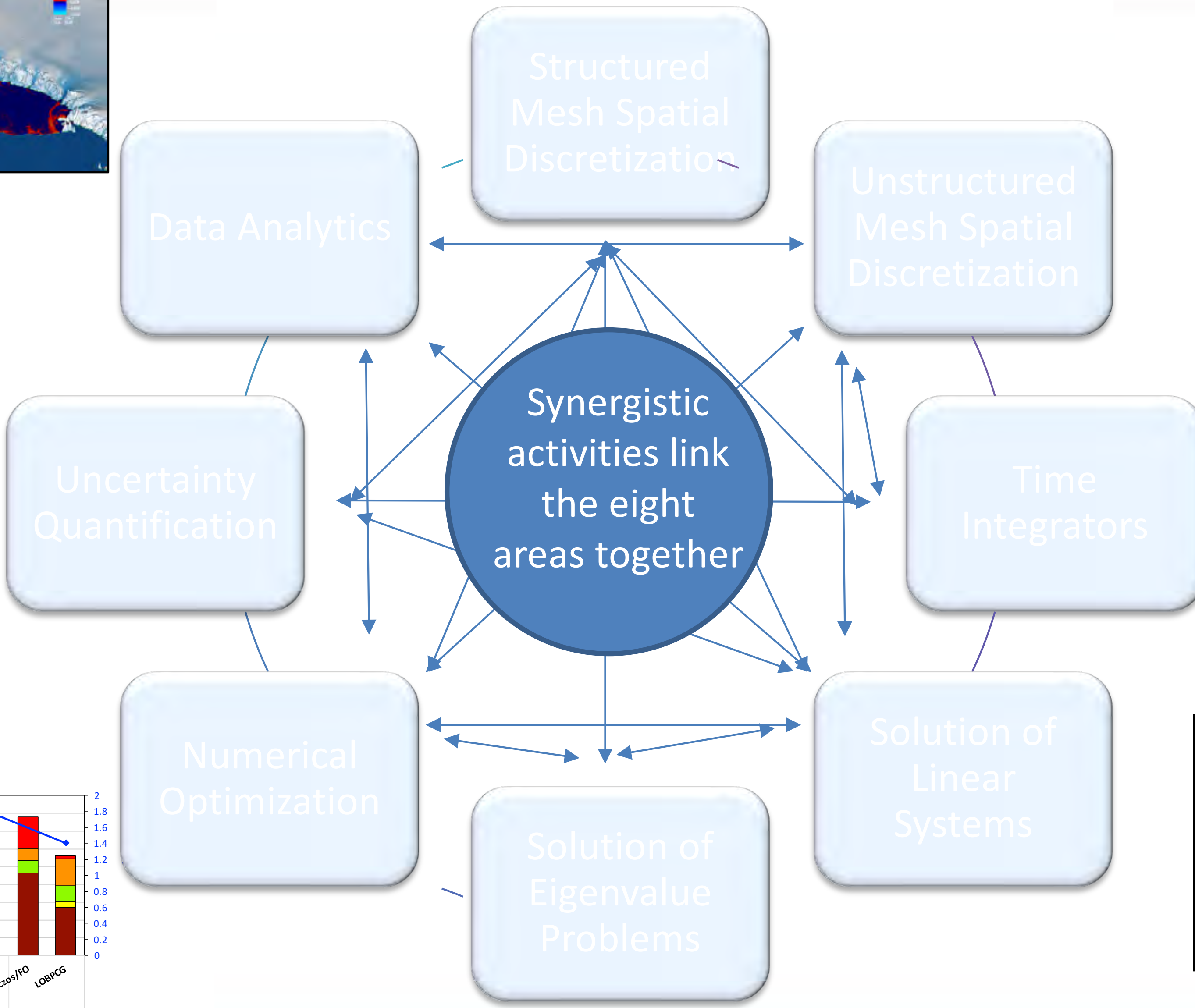
- Legendre systems: $m = O(s^2)$ instead of $O(s^{2.58})$ as in unweighted l_1.
- Chebyshev systems: $m = O(s^{1.58})$ instead of $O(s^2)$ as in unweighted l_1.

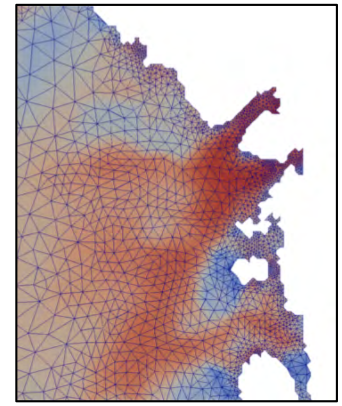
A. Chkifa, N. Dexter, H. Tran, and C. Webster, *Polynomial approximation via compressed sensing of high-dimensional functions on lower sets*. **Math. Comp.** (2017) https://doi.org/10.1090/mcom/3272

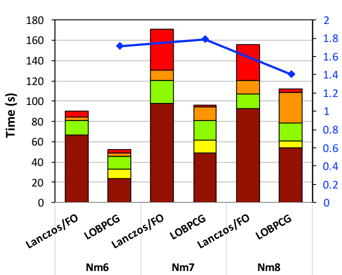
Eight core technology areas: Synergistic Activites

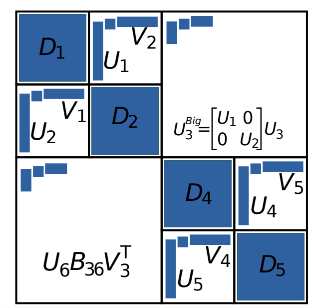












Synergystic activities will results in new capabilities or higher efficiencies

New Capabilities

- Optimization under uncertainty
- Discrete and multi-objective optimization for data analytics
- In situ simulation on unstructured meshes

Higher Efficiency

- Leverage multiple right hand sides from optimization and UQ ensembles in linear and nonlinear solvers
- Adaptivity in the spatial and stochastic space in UQ on unstructured grids;
- Dynamic UQ load balancing
- In situ simulation on unstructured meshes

The FASTMath organizational structure follows from the core technical areas

Institute Management
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Esmond Ng, LBNL, Deputy Director

Institutional POCs
T. Munson, ANL
E. Ng, LBNL
L. Diachin, LLNL
R. Archibald, ORNL
M. Shephard, RPI
K. Devine, SNL

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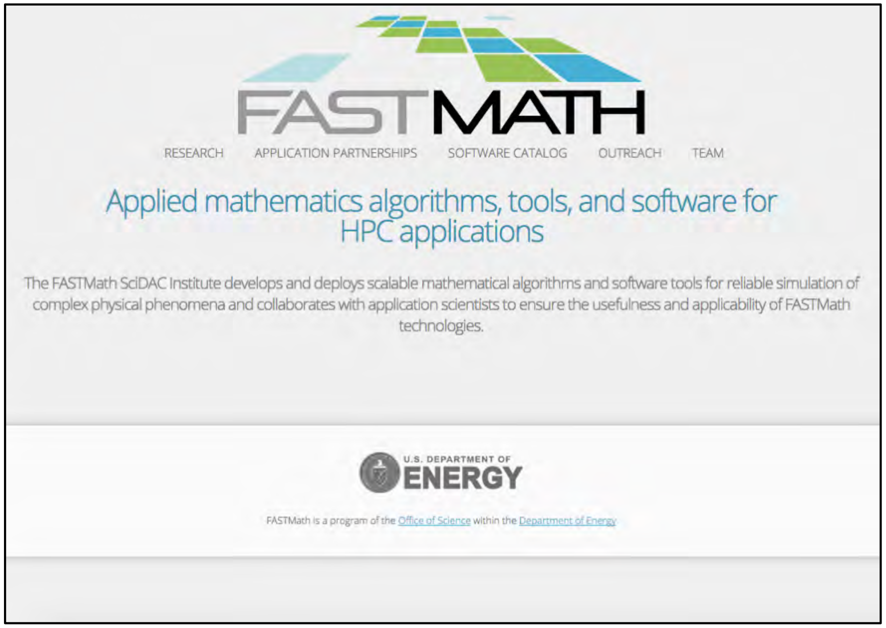
  – www.fastmath-scidac.org



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